A Software Environment for Developing Complex Multiphysics Applications

http://www.esc.sandia.gov/sierra.html

http://www.cfd.sandia.gov/sierra.html

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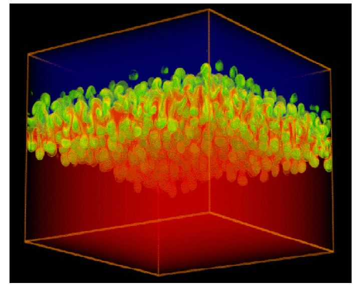
DOE's Accelerated Strategic Computing Initiative (ASCI)

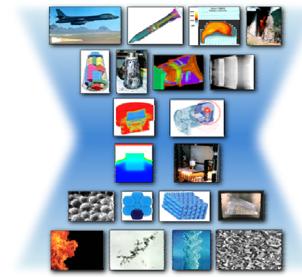
Computers

Develop massively parallel, high performance computers to achieve the ASCI 100 TeraOps computing goal by 2004



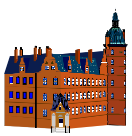
Applications Codes

Modify and develop codes to achieve the speedup's and improvements necessary to perform full physics simulation



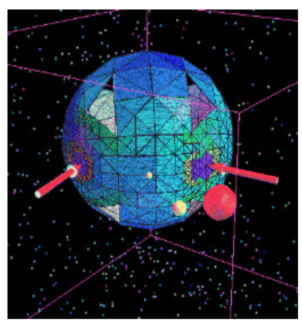
Verification and Validation

- Provide the tools methodologies and data to ensure that high-end simulation capabilities reflect reality
- Establish confidence in the predictive capabilities of ASCI tools



Alliances

Partner with universities, to solve computing and simulation challenges



Problem Solving Environments

Make the full-physics codes user friendly to weapons analysts including set-up of large scale problems, transferring and storing tera-byte size files, and 3D visualization on the desktop of these tera-byte size files

isCom^2

- Implements secure Tera-scale computing across 1000s of miles
- Integrate information and simulation
- Install distributed security and resource management

SIERRA Concept

Applications share a single framework which provides common capabilities

- Simplify utilization of ASCI supercomputers
- Consolidate common capabilities
- Eliminate redundant development and maintenance
- Encourage architecturally similar applications

Application developers work in a common software development environment

- Uniform access to ASCI resource (program elements)
- Utilize a common source code repository
- Coordinate development efforts
- Consolidate the set of software development tools
- Share software development processes

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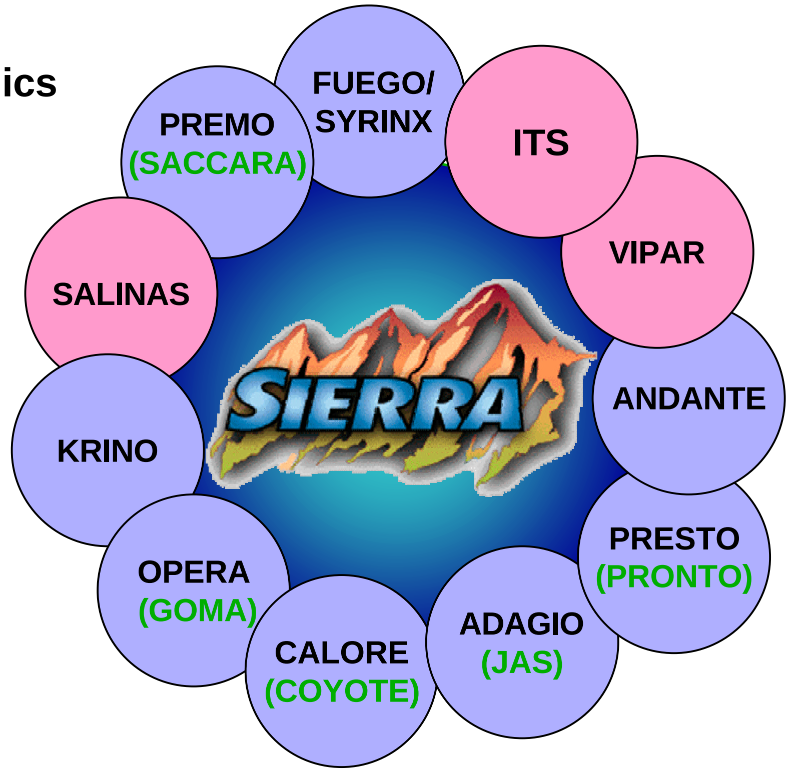
Migration of Sandia Application Codes

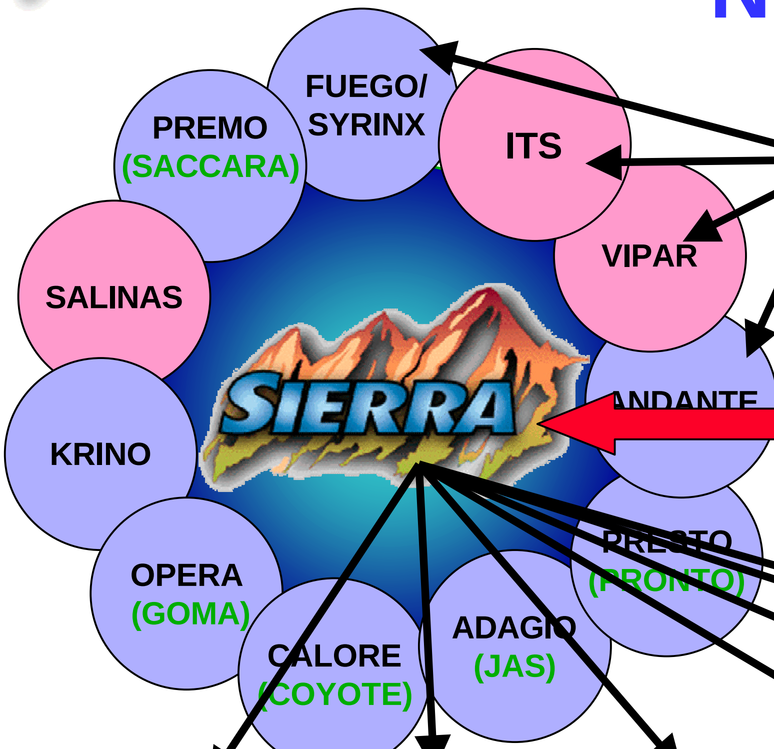
VIPAR	Parachute performance code, vortex method coupled with transient dynamics
PRONTO	Transient dynamics Lagrangian solid mechanics
JAS	Quasi-static solid mechanics
COYOTE	Thermal mechanics with chemistry
GOMA	Incompressible fluid mechanics with free surface
SALINAS	Structural dynamics
SACCARA	Compressible fluid mechanics
ITS	Radiation transport

Current stand-alone codes



Current and future SIERRA-based codes

Minimize Cost for Development, Maintenance, and Porting to New ASCI Resources

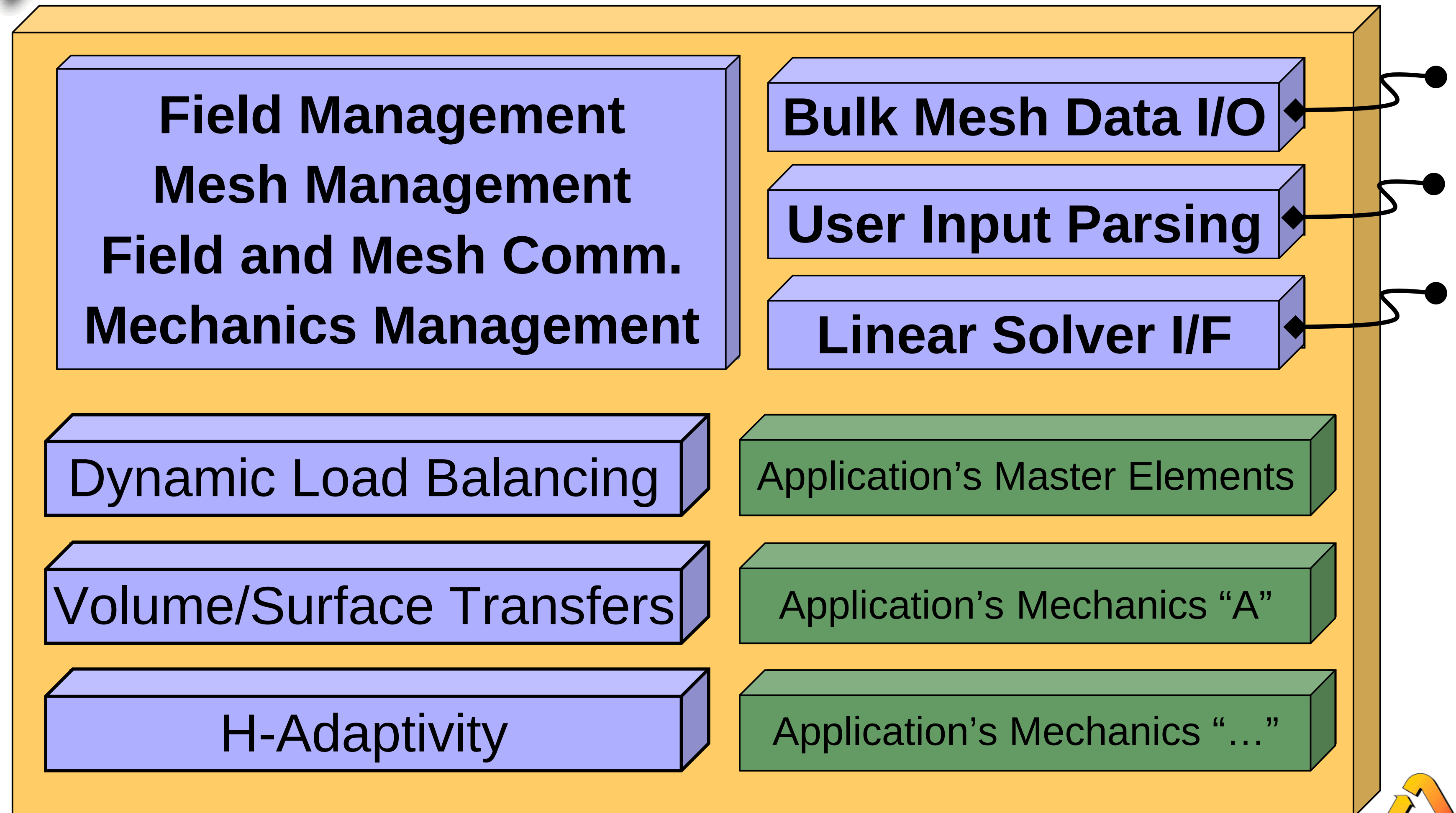


Physics dependent algorithms (i.e. mechanics)

Physics independent algorithms
Computer dependent capabilities

SNL Red Janus | LLNL Blue Pacific | LANL Blue Mountain | SNL Cplant | LLNL White | LANL Q | SNL Red Storm

SIERRA Framework Capabilities



Finite Element Services

- **Fully unstructured mesh**
  - Nodes, Edges, Faces, Elements
- **Fields associated w/ interpolation, integration**
- **<u>Master Element Interface</u>,** *not implementation*
  - Element topology
  - Parametric coordinate mapping
  - Interpolation
  - Numerical integration

  ⇒Implemented and shared by application developers

Mesh Management

- **Unstructured mesh**
  - Arbitrary mesh object connections
  - Overlay element topologies (hex, tet, quad, …)
- **Dynamic creation/deletion of mesh objects**
- **Subsets of mesh objects**
  - Define by part, material type, boundary, constraint, …
  - Define unions and intersections of subsets
  - Apply algorithms to specified subsets
- **Fully distributed mesh data structure**

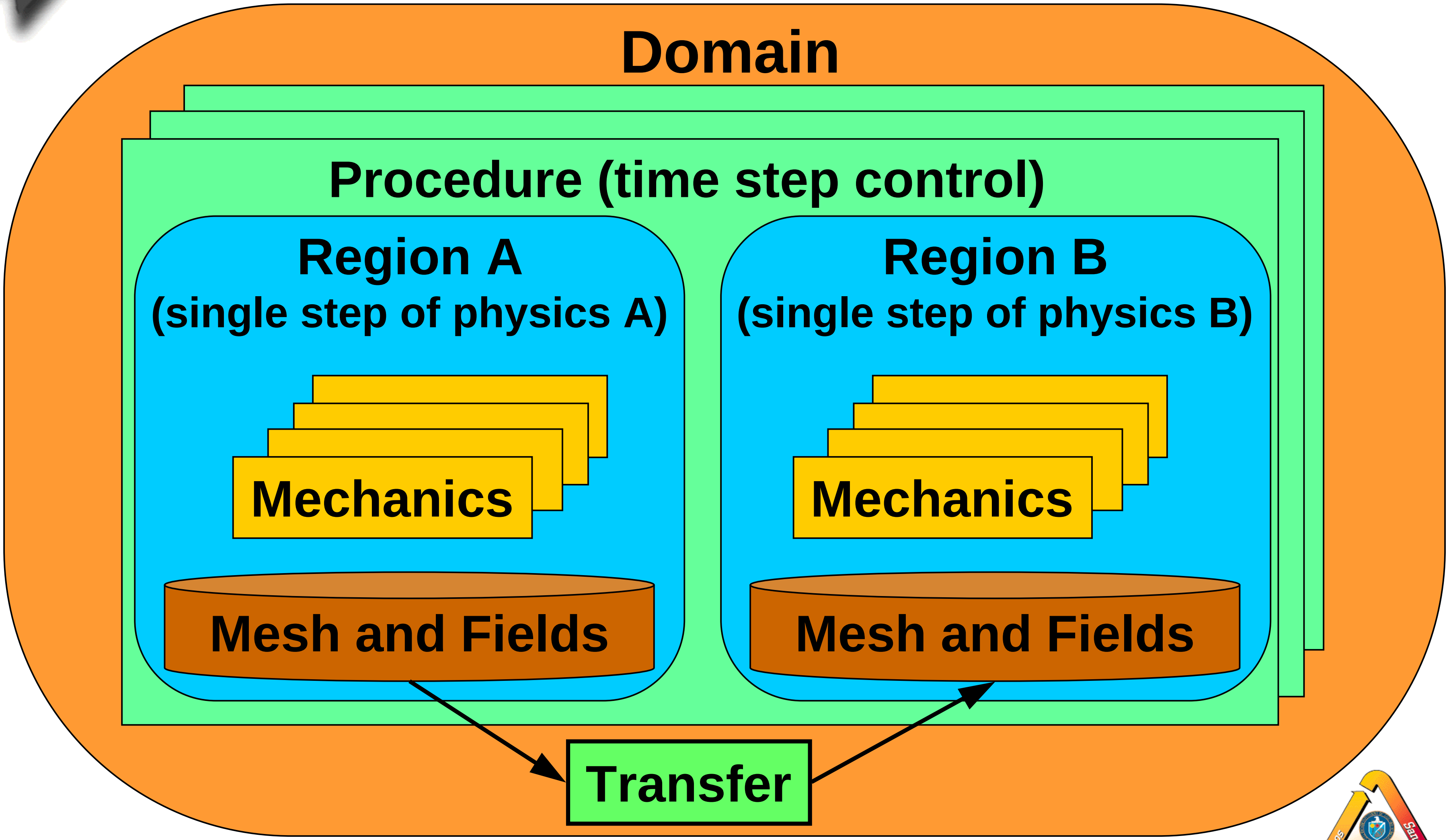
Field Management

- **Application defined fields (a.k.a. variables)**
  - Text name
  - Type (int, real, vector, full tensor, symmetric tensor, …)
  - Aggregate types (e.g. collection of material variables)
  - Optionally associated with a master element (interpolation field, integration field)
  - **Associated with a subset of mesh objects**
- **Memory management for field values**
  - Only allocate for the **subset** of mesh objects
  - (field , mesh-object $\in$ subset) $\rightarrow$ allocated value
  - (field , mesh-object $\notin$ subset) $\rightarrow$ NO value

Mechanics Management

- **Mechanics Modules (supplied by Application)**
  - Algorithms, fields and parameters for a "physics"
  - Applied to specified subset of mesh objects
  - Parameters for each subset (material properties, boundary values, …)
  - Uses zero-to-many master elements
- **Multiple mechanics modules**
  - Coupled via shared fields and mesh subsets
  - Hierarchical nesting of mechanics modules, e.g. a material mechanics nested within an element mechanics

Mechanics Module Hierarchy



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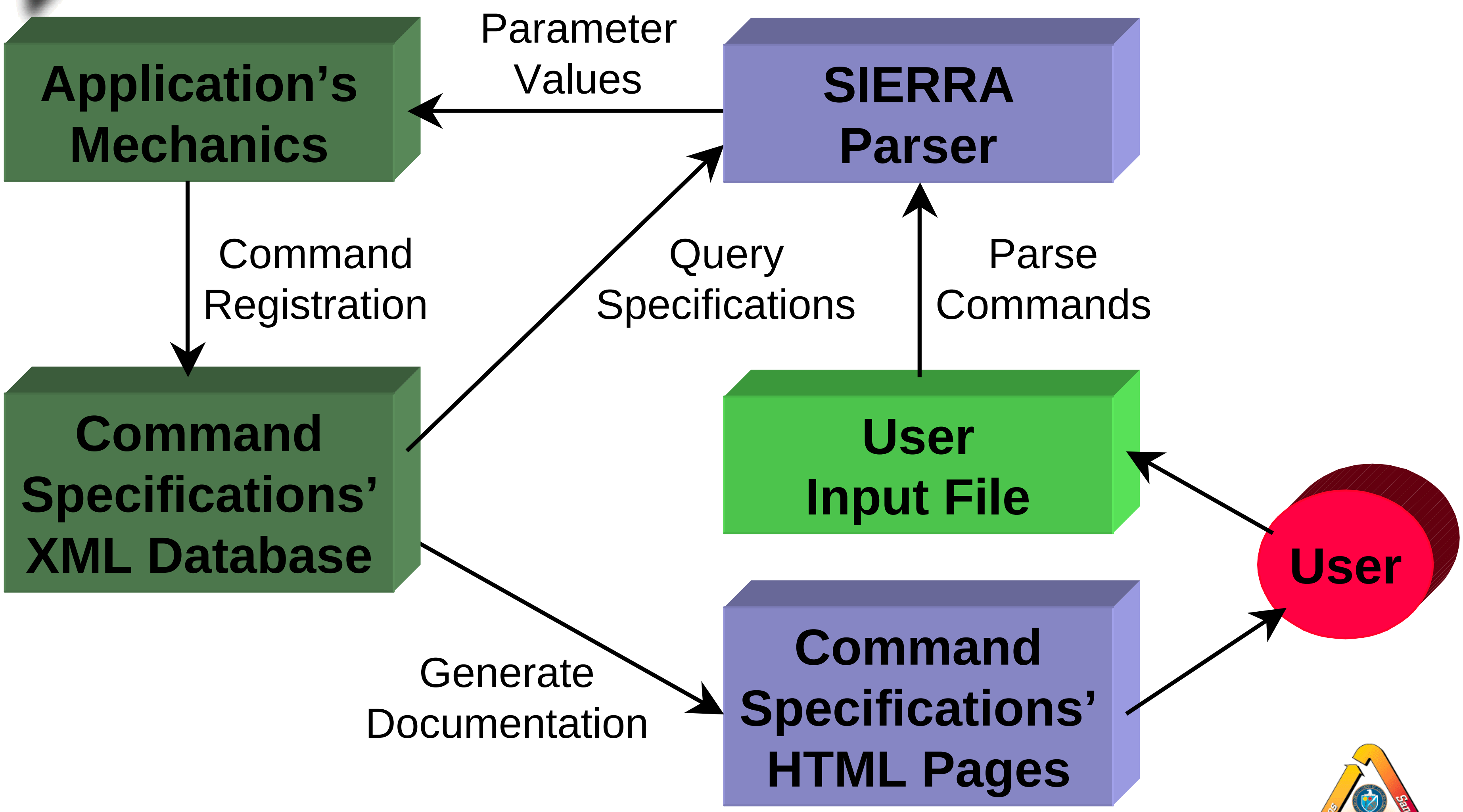
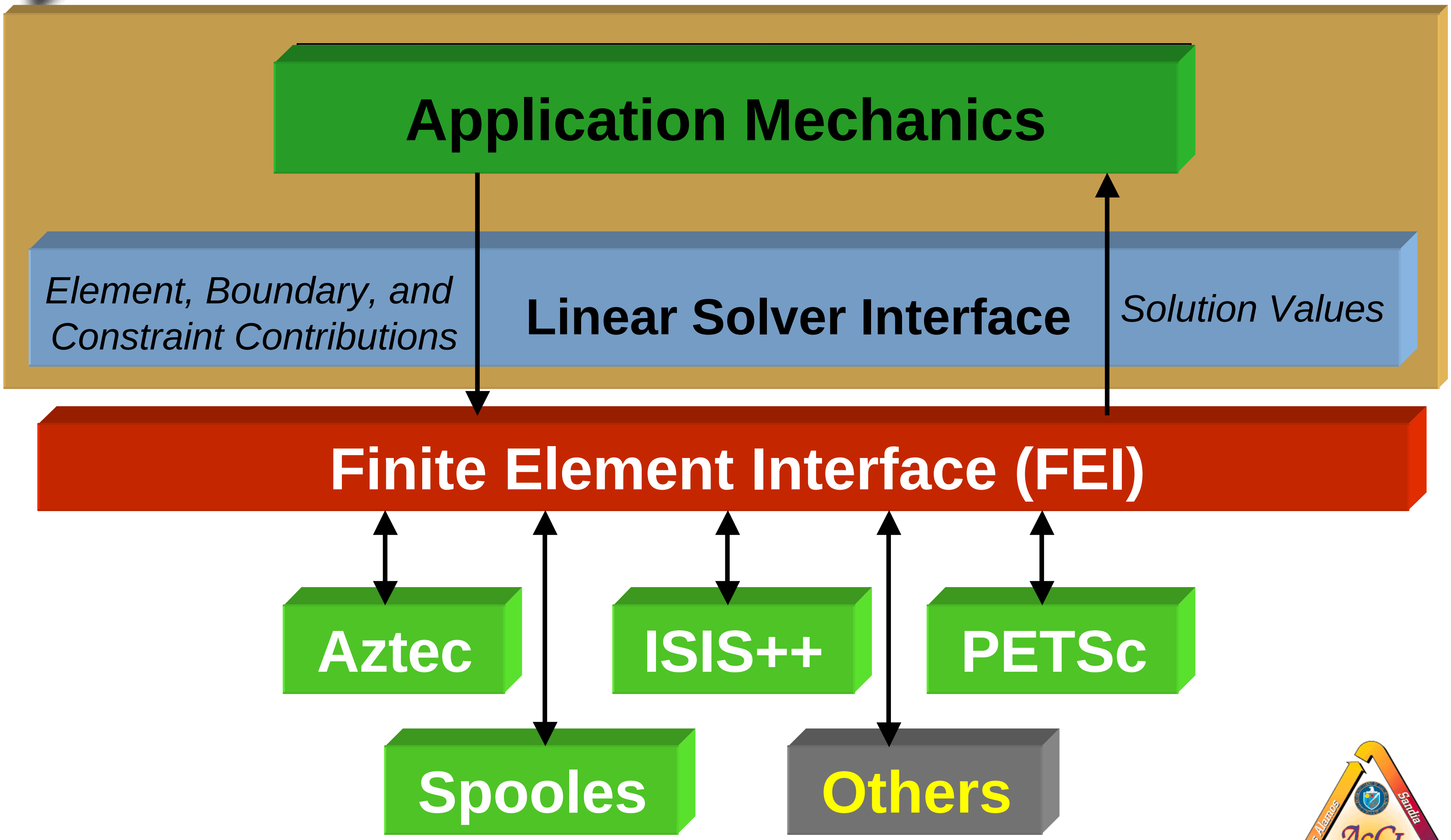
Bulk Mesh Data Input/Output

- **Bulk Mesh Data Input/Output Services**
  - Parallel IO for mesh topology and field values
  - Output files for post processing / visualization
  - Restart
- **Simple application interface, specify:**
  - What files for input/output
  - Which mesh subsets and fields
  - When to output
- **Transparent access to multiple file formats**
  - ExodusII (SNL), DMF (ASCI Tri-Lab), …

User Input Parsing



Linear Solver Interface



SIERRA Framework Advanced Capabilities

- **Dynamic Load Balancing**
  - Automatically balance computational load among processors of a massively parallel computer
  - Critical for efficient use of ASCI computers
- **Volume/Surface Transfers**
  - Couple independently developed mechanics
  - Critical to solve complex multiphysics problems required for Stockpile Stewardship
- **Adaptivity (of mesh)**
  - Automatically improve accuracy of solution
  - Critical for confidence in problem solutions

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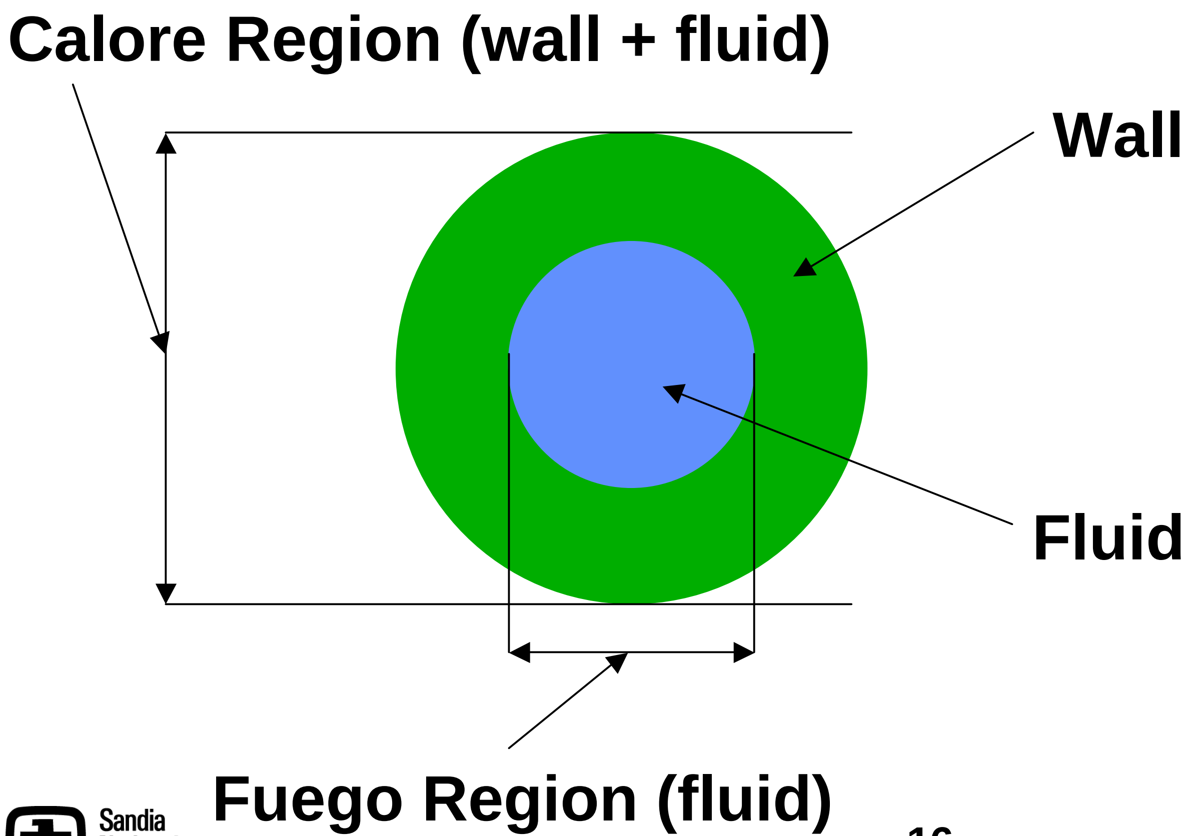
Coupled Fluid/Thermal Problem Layout

- **Applications divided over wall and fluid**
  - Calore solves for temperature in all regions
  - Fuego solves for velocity and delivers to Calore



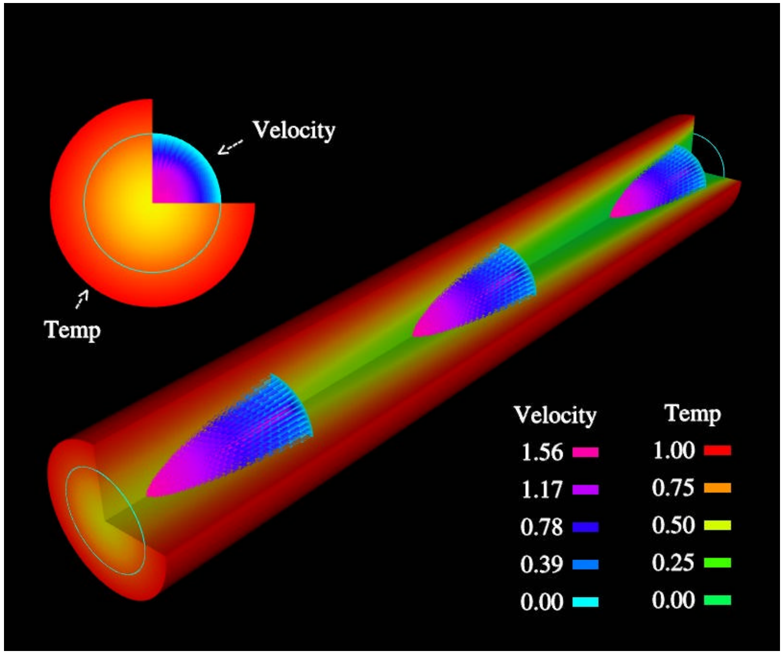
Coupled *Calore/Fuego* (Thermal/Flow) Pipe Flow Problem

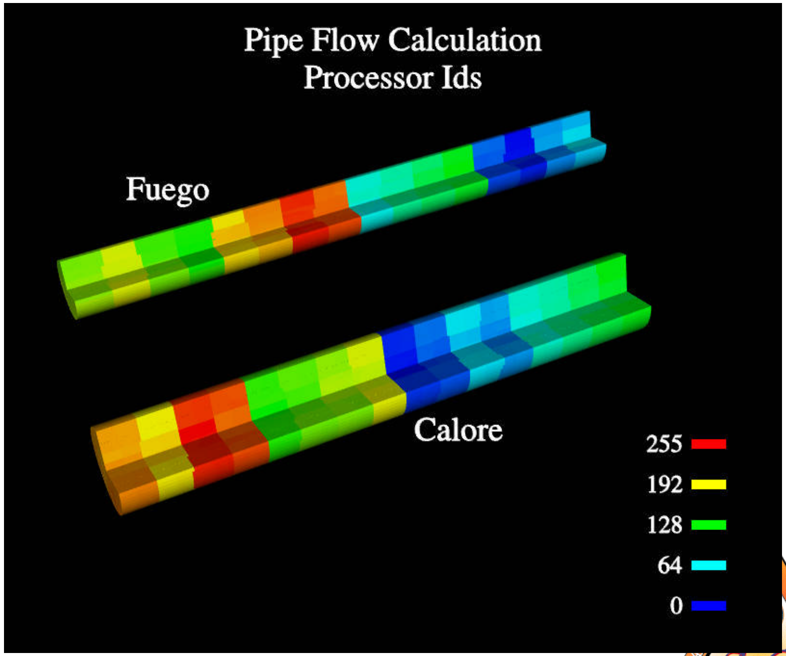
Calore

- Mesh both pipe and fluid
- *Transfer* fluid temperature to Fuego

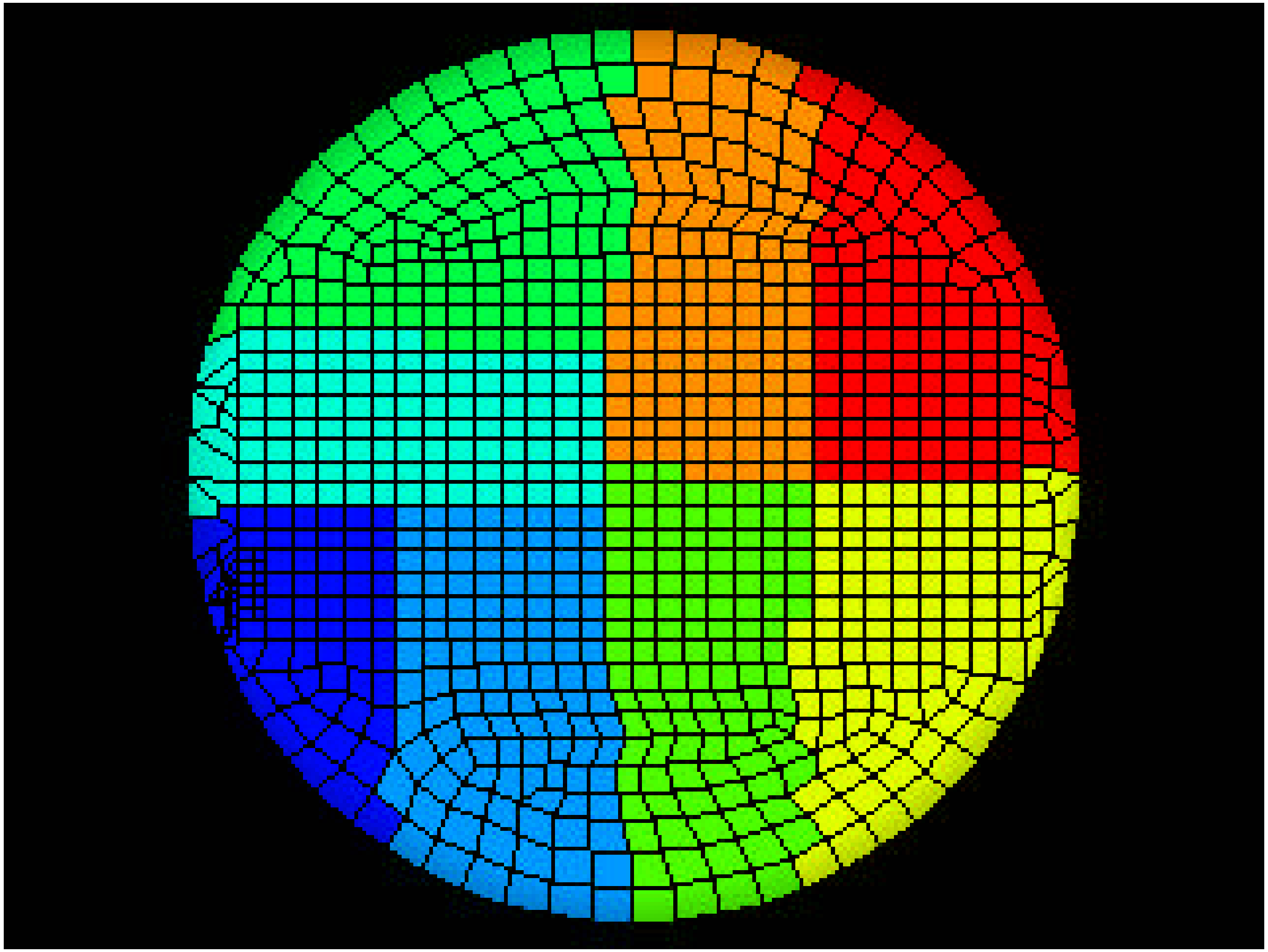
Fuego

- *Different* mesh for fluid
- *Transfer* fluid velocity to Calore





Electron Beam Rastering
8 Proc Dynamic Load Rebalancing



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Summary

- **SIERRA Framework Services**
  - Distributed Mesh, Field, and Mechanics Management
  - Communications, Solver Interfaces, I/O, Input Parsing
  - Dynamic Load Balancing, Transfers, H-Adaptivity
- **SIERRA Software Development Services**
  - Configuration Management & Regression Testing
  - Requirements Management & Verification Testing
- **Minimize total life-cycle cost for the set of SIERRA-based ASCI Application codes**

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Fault Tolerance in FY03 Requirements

- Gracefully handle application faults
  - Iterative solver fails to converge
  - Distorting element inverts (negative jacobian)
  - Non-catastrophic bug, e.g. C++ exception thrown

- Provide application with an opportunity to
  - Recover, e.g. roll-back current time step
  - Gracefully exit, e.g. clean post-mortem data dump

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Fault Tolerance in FY03 Concept

- Introduce parallel “exception” handling capability in the SIERRA Framework
  - Register exception code with a handler (callback function) ~ signal handlers
  - Set exception code on any processor
  - Next collective communication call the associated handler on every processor
- C++ exception catch blocks can set the exception code
  - parallel exception handling if caught before the next collective communication

Fault Tolerance in FY03 Implementation

- **MPIH: Collective message-passing w/handlers**
  - **Developed by Dr. Robert van de Geijn / UT-Austin under SNL contract**
  - **Specifications from SNL / Carter Edwards**
  - **Uses “pure” MPI, no machine dependent signals**
  - **Low overhead and no extra message data!**
  - **Includes the essential sparse all-to-all variable length message collective operation**
- **MPIH status**
  - **Currently undergoing software quality assurance (SQA) porting and testing**